Paradigm Shift for Resonance-Region Uncertainties

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Two issues for resonance covariances

- **File 32 is difficult to deal with**
  - **Size is often very large**
  - **Calculating the evaluated cross section covariance matrix from File 32 is complicated**

Save this topic for the end of the talk

- **The resonance parameter covariance matrix cannot convey complete information**

The main topic for this talk

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Synopsis of the issue

- **R-matrix analysis automatically produces a resonance parameter covariance matrix** = RPCM
- **From the resonance parameters, we reconstruct point-wise cross sections**
  - **Also multigroup cross sections**
- **From the RPCM, we construct the covariance matrix for the evaluated cross sections** = ECM
- **The ECM constructed using only the RPCM is generally regarded as "too small"**

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Why is the ECM too small?

- **It is not possible for RPCM to convey complete information concerning ECM**

Reasons will be discussed separately…

- **Several reasons for this**
  - **Computation of RPCM is based on assumptions which are not fully valid**
  - **Bayes' equations (or least-squares equations) contain no information about goodness-of-fit**
  - **Experimental data base is not unique**

Assumptions on which RPCM is based:

1. **R-matrix theory is correct**
   - **All resonances are included**
     - **Even very small invisible resonances**
   - **All spin assignments are correct**
     - **No ambiguity**
   - **No direct components or other extensions exist**
   - **Everything is calculated correctly**
     - **No bugs in the code**

These assumptions are all reasonable but imperfect

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Assumptions, continued:

2. **All experimental conditions are properly understood and included in the analysis**
   - **Corrections are accurately made for**
     - **Doppler and resolution broadening**
     - **Multiple-scattering corrections**
     - **Normalization and background**
     - **Etc.**
   - **Everything is calculated correctly**
     - **No bugs in computer codes, no omissions in theory**
   - **All experimental uncertainties are described correctly**
   - **No discrepancies exist between data sets**

These assumptions are reasonable but imperfect

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Conjecture: Why is the ECM too small?

- It is not possible for RPCM to convey complete information concerning ECM

- Several **reasons** for this
  - Computation of RPCM is based on assumptions which are not fully valid
  - **Bayes' equations (or least-squares equations) contain no information about goodness-of-fit**
  - Experimental data base is not unique

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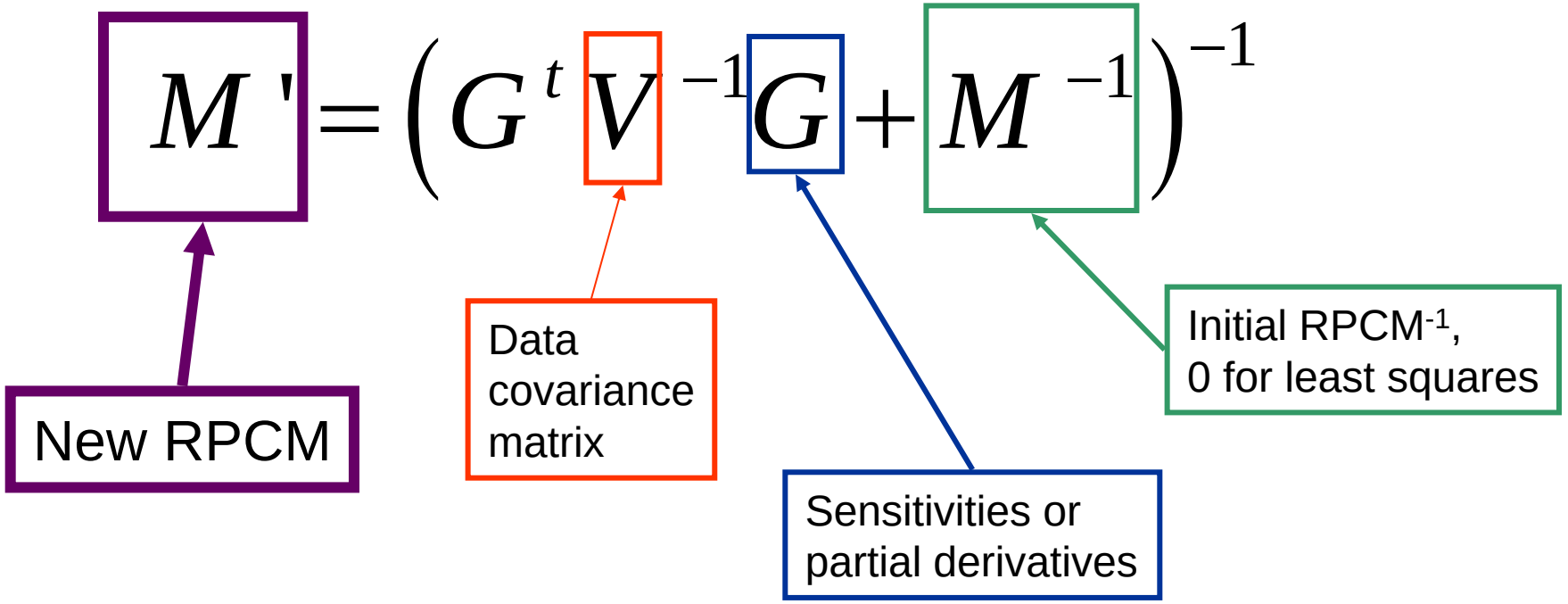
Bayes' Equations for RPCM



Appearing nowhere in this equation: the difference between theory and measurement

Conjecture: Why is the ECM too small?

- It is not possible for RPCM to convey complete information concerning ECM

- Several **reasons** for this
  - Computation of RPCM is based on assumptions which are not fully valid
  - Bayes' equations (or least-squares equations) contain no information about goodness-of-fit
  - **Experimental data base is not unique**

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Experimental data base

- **Evaluator constructs a "consistent" experimental data base**
  - **Based on results of preliminary analyses**
  - **Normalization = 1, background = 0**
    - **uncertainties included as SAMMY PUPs**
- **This data base is not unique**
  - **Depends on ability of evaluator to extract information from publications (often incomplete)**
  - **Systematic uncertainties should reflect this fact**

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Logical conclusion

- **The resonance parameter covariance matrix alone cannot provide complete information regarding the uncertainty on the evaluated cross sections**
- **Something else is needed**

- **It is not obvious how one quantizes the effects described above**

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What can be done?

- **Historically**
  - **Increase the RPCM in rather arbitrary fashion**
- **Currently**
  - **Still doing something like that**
- **Future**
  - **Add realistic components to the ECM**
    - **One component from RPCM**
    - **Other components from other effects**

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Other components

- **Two important and easy-to-implement possibilities**
  - **Normalization**
    - **Value a = 1, uncertainty $\Delta a \sim 0.03$**
  - **Background**
    - **value b = 0, uncertainty Δb, perhaps energy-dependent**
- **These may not directly represent the effects described earlier, but they should be a good first approximation**

One option for inclusion in ENDF

- **Use File 33 to introduce normalization and background uncertainty**
  - **No format changes required**
  - **Doro Wiarda is working on this possibility**
    - **Preliminary results are promising**
    - **Potential problems exist because of derived quantities (elastic = total – everything else)**

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Preliminary results …

- **^{55}Mn capture cross section, expressed in arbitrary group structure**
- **Two versions**
  - **With only RPCM**
  - **With combination of**
    - **RPCM**
    - **Normalization uncertainty = 0.03**
    - **Background uncertainty varies with energy**
      - **Lowest = 0.8 % of average cross section**
      - **Highest = 15 %**
- **(No higher-energy information is included in these plots)**

Proof-of-principal only, not a realistic case

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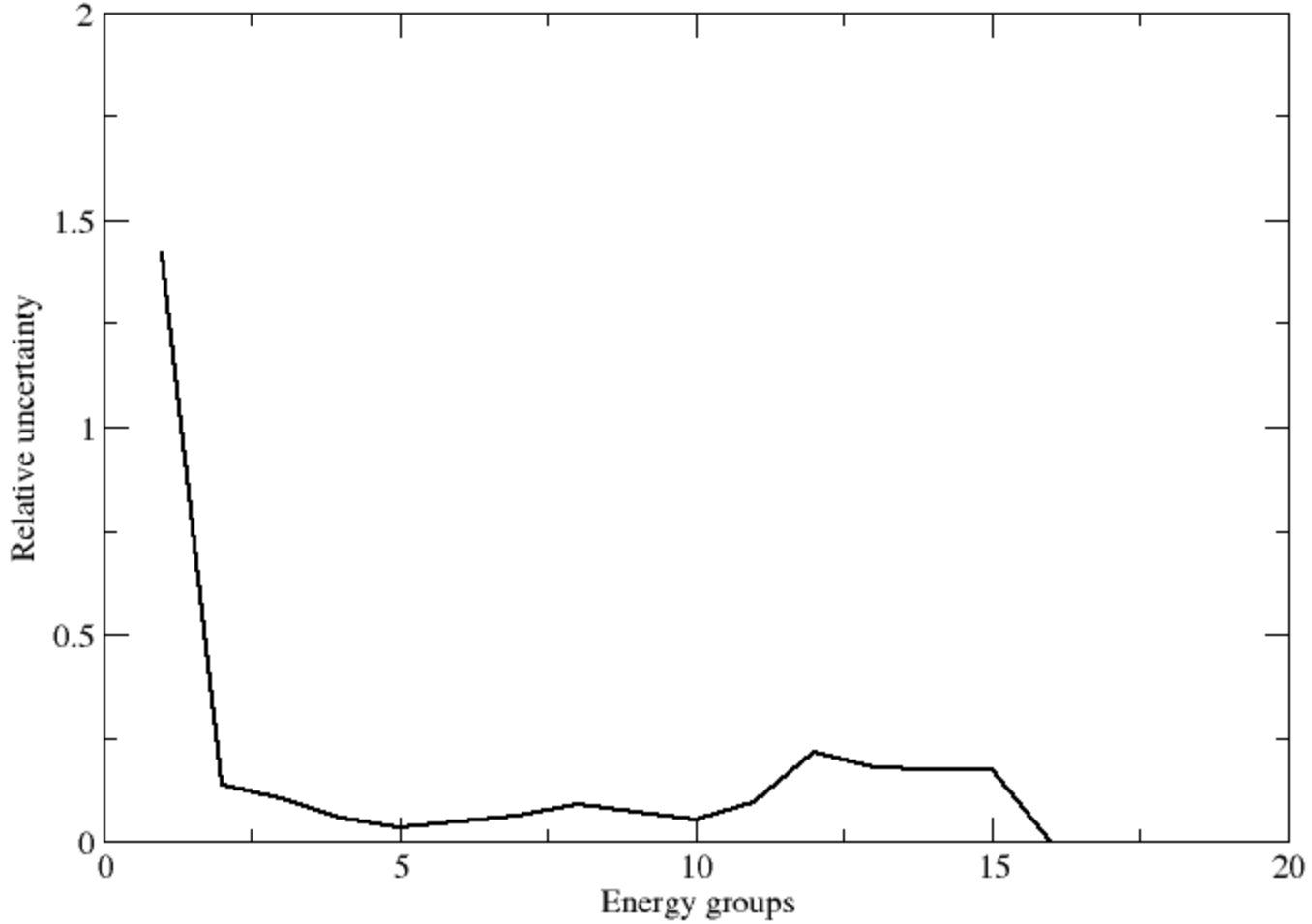
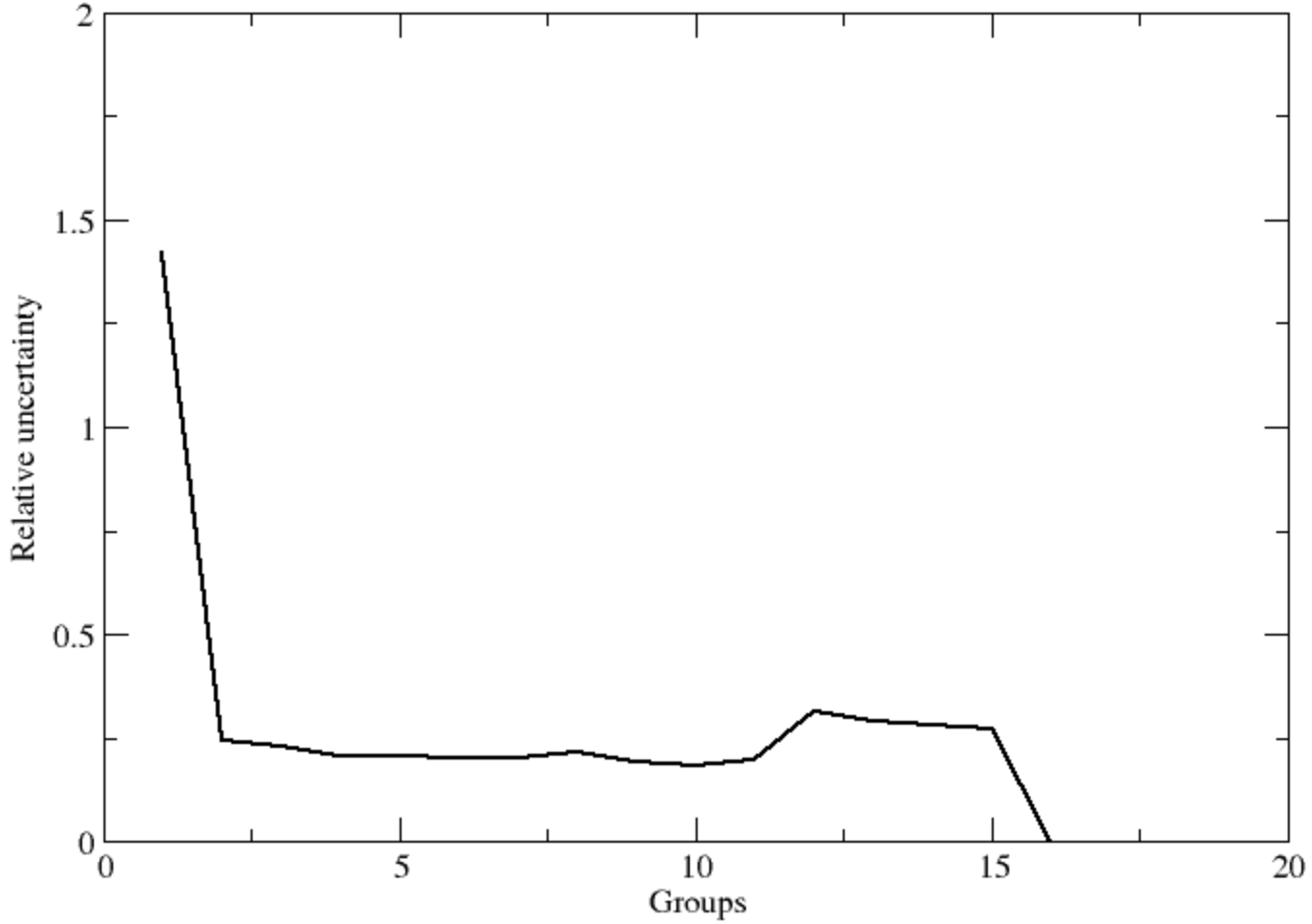
Relative uncertainty, with only RPCM



Relative uncertainty, with RPCM + norm + background unc.



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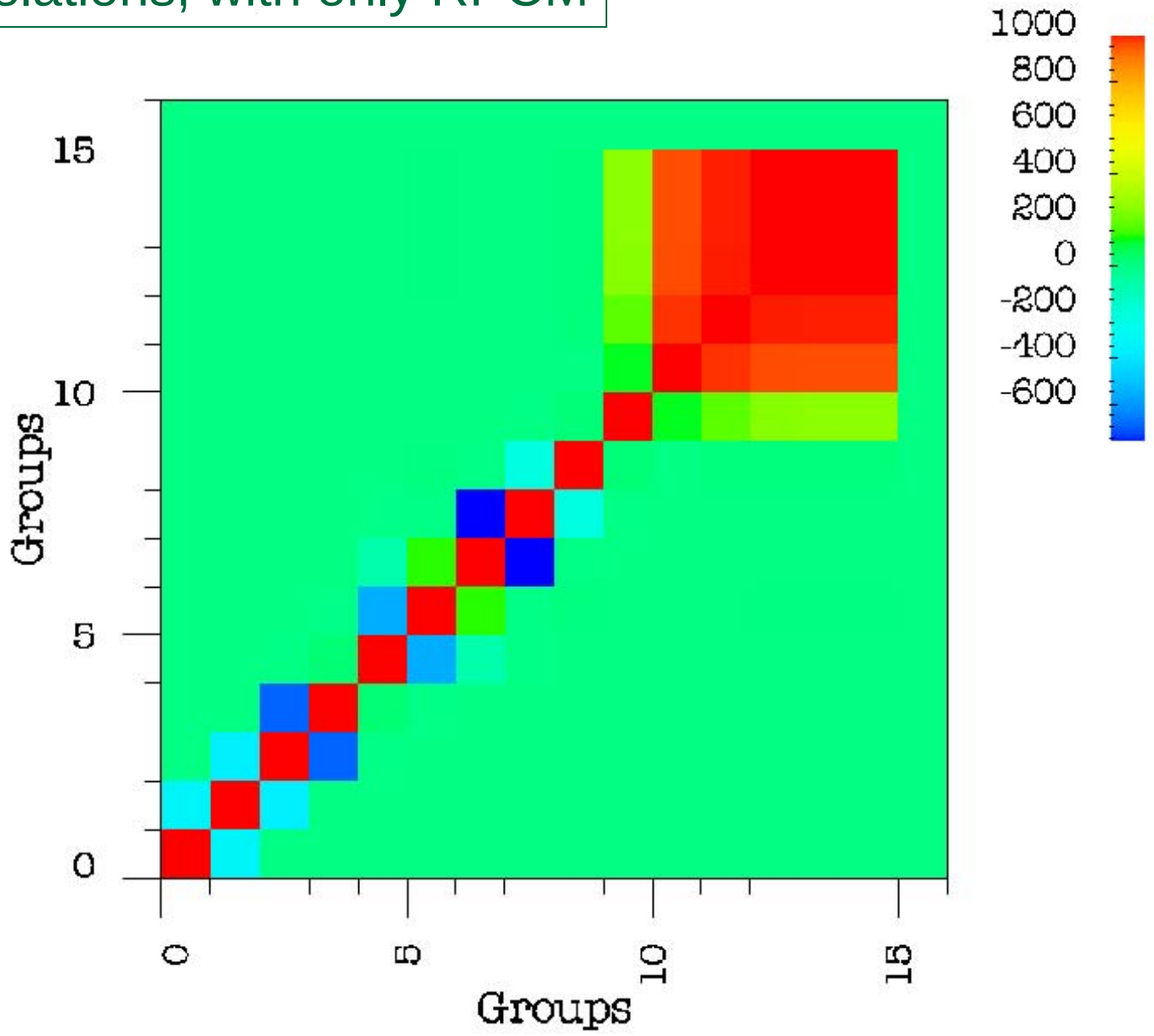
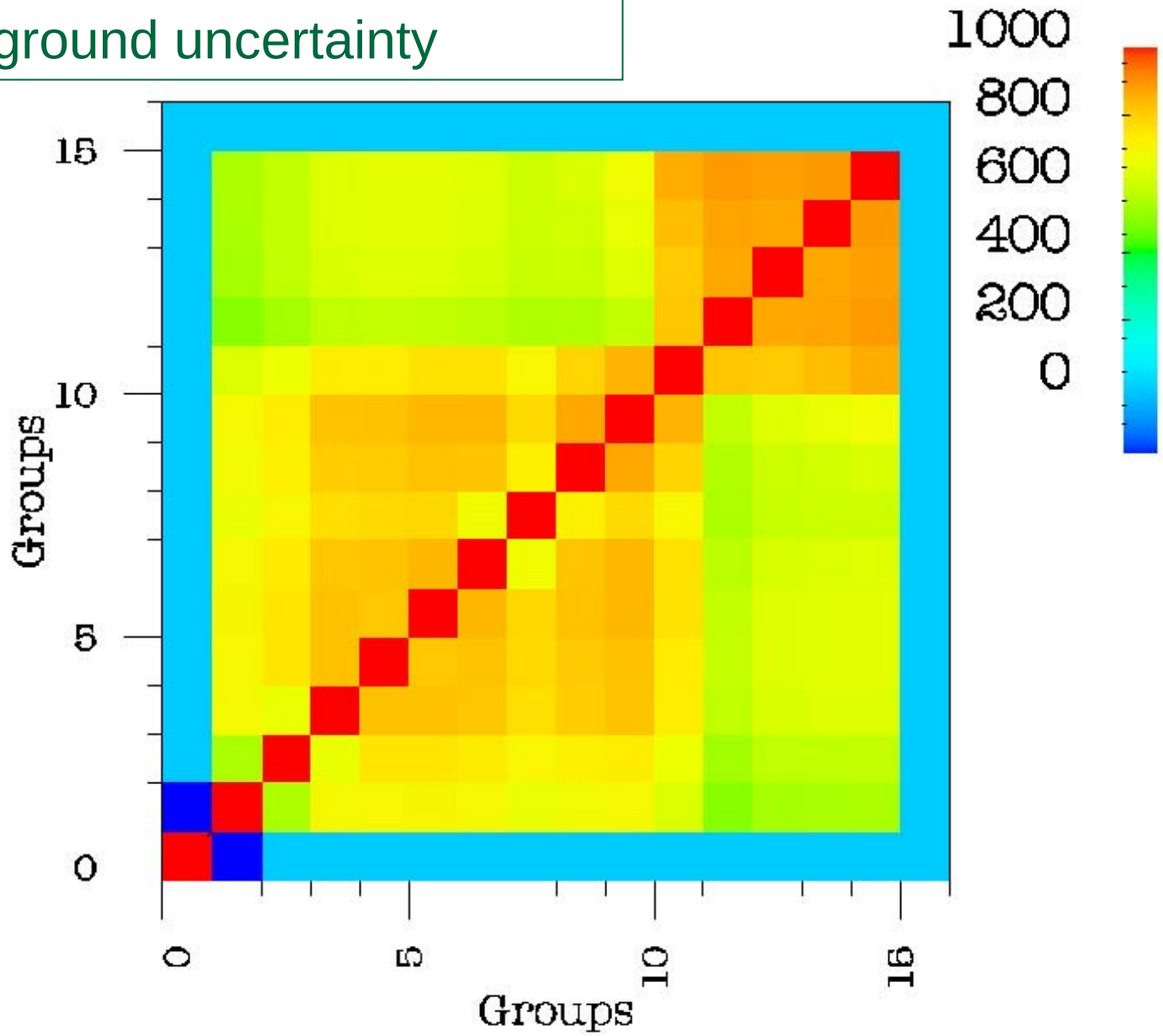
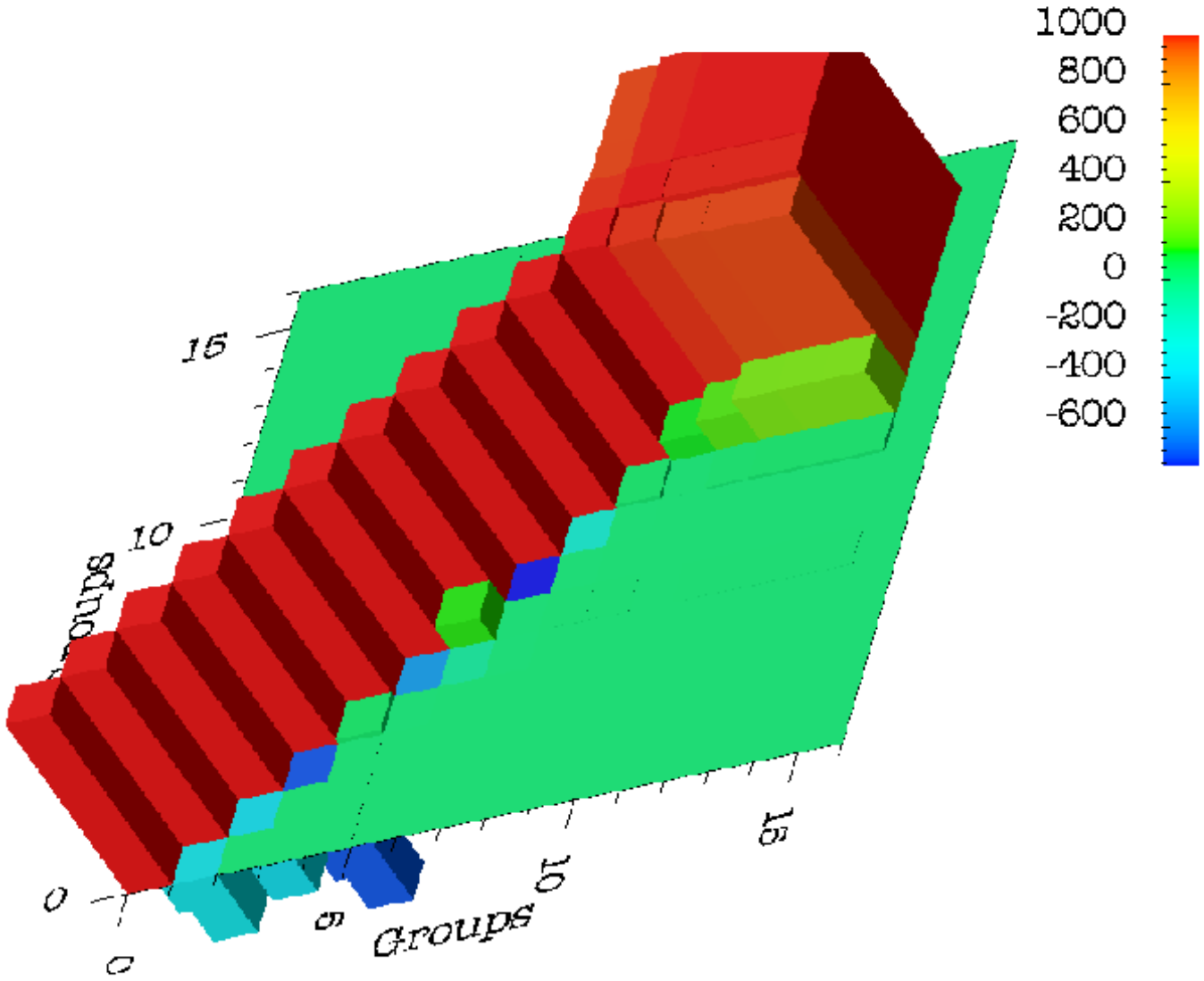
Correlations, with only RPCM



Correlations with RPCM + norm + background uncertainty



Another view of correlations with only RPCM



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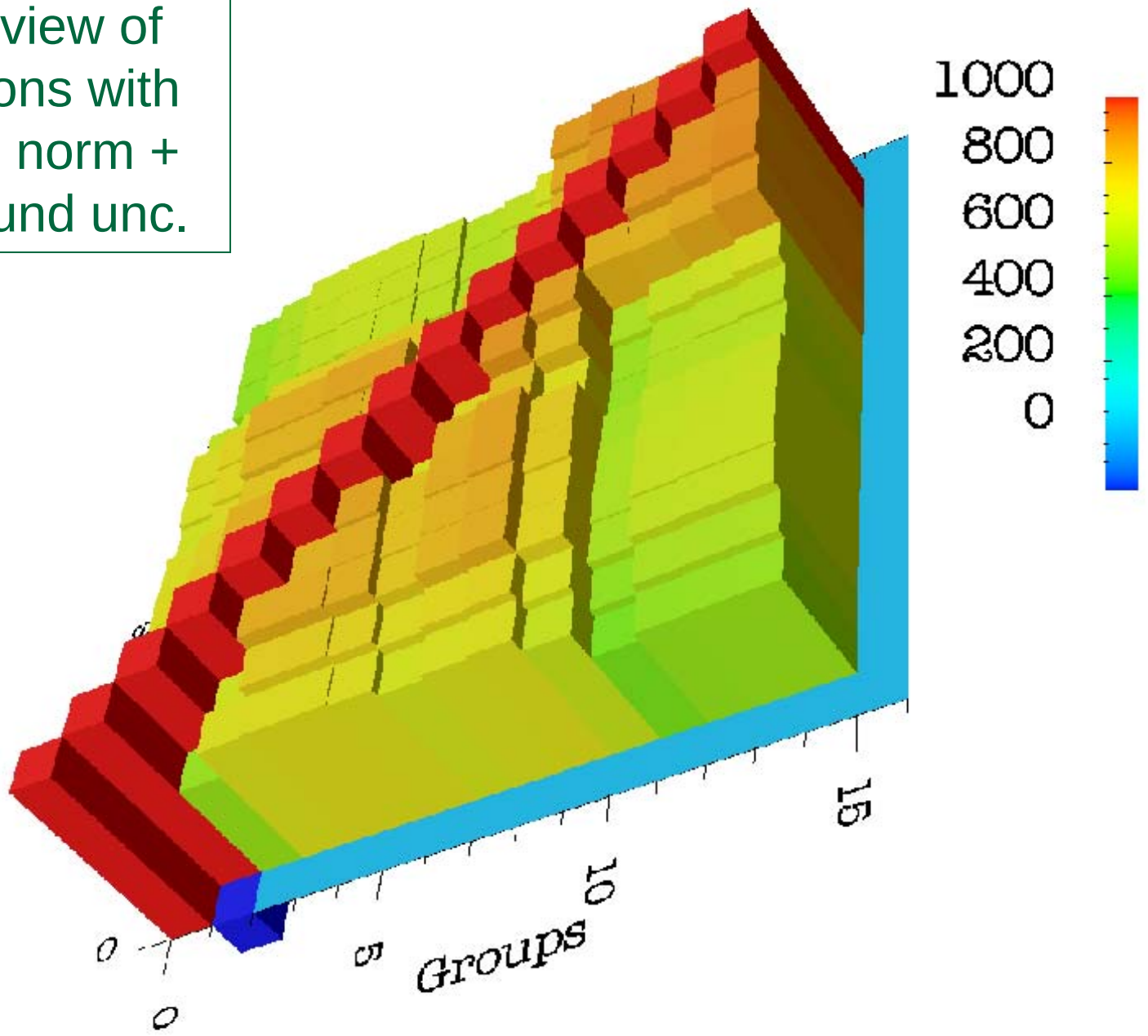

Another option for inclusion in ENDF

Luiz Leal, Goran Arbanas, Doro Wiarda

- **Add RPCM plus other components prior to writing into ENDF files**
  - **Judiciously choose energy grid for storage of the complete ECM in File 33 of ENDF**
    - **Grid is chosen to convey maximum information for the nuclide – depends on level spacing, etc.**
    - **Grid must be tested to be sure that little information is lost**
      - **Test ➔ compare to results generated using full ECM**
  - **File 32 would not be needed**
    - **This avoids the problems of storing too-large arrays**

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Conclusions

- **Paradigm shift may be necessary**
  - **Cannot expect the resonance parameter covariance matrix to convey all information about evaluated cross section uncertainties**
- **First-order effects should not require ENDF format changes**
- **File 33 can sometimes be used alone to convey the complete point-wise covariance matrix**
  - **When the energy grid is sufficiently fine and tailored to the specific nuclide**

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The end

The following slides show the same figures as above, but in a different group structure (AMPX standard 44-group structure)

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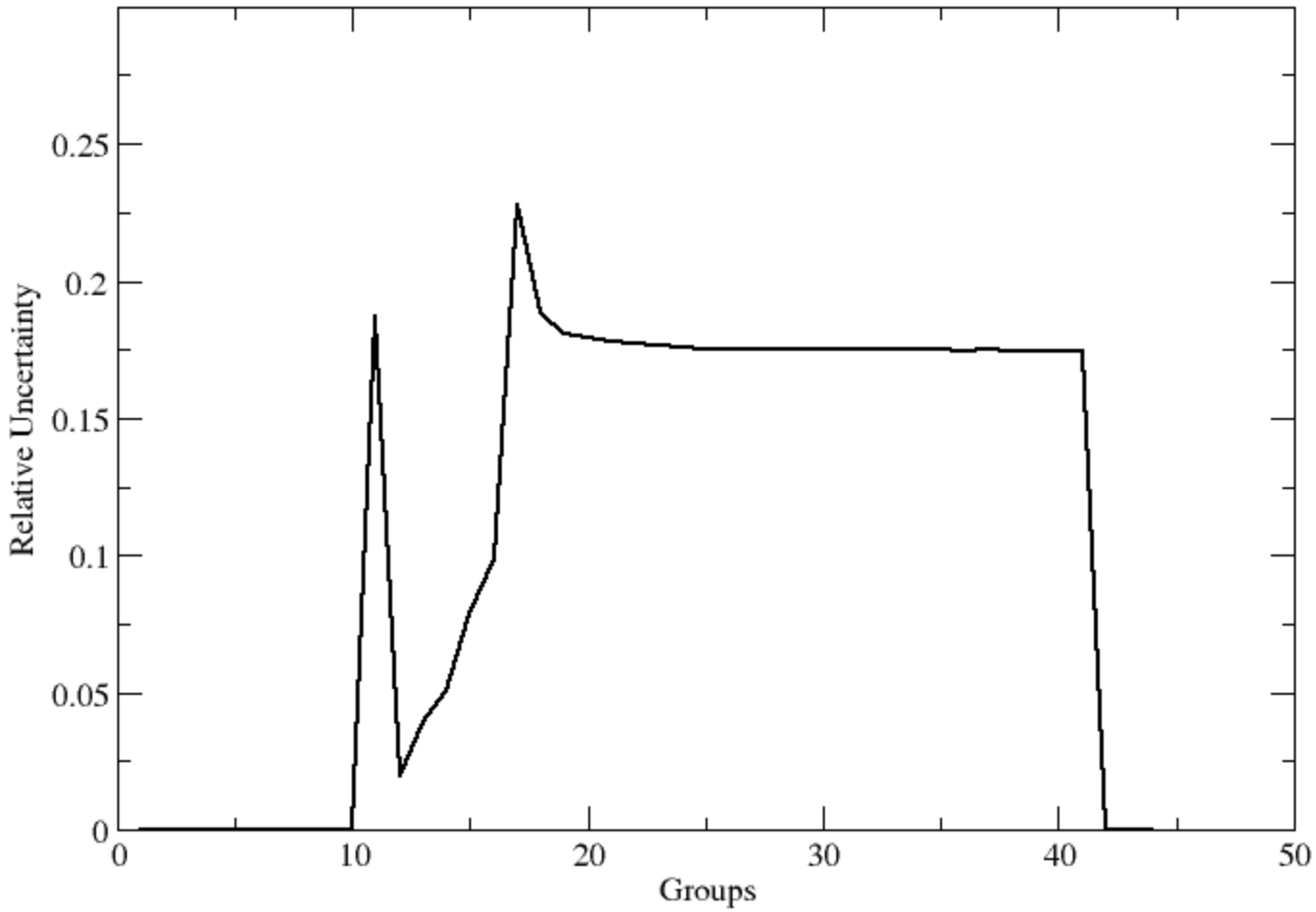
Relative uncertainty, with only RPCM



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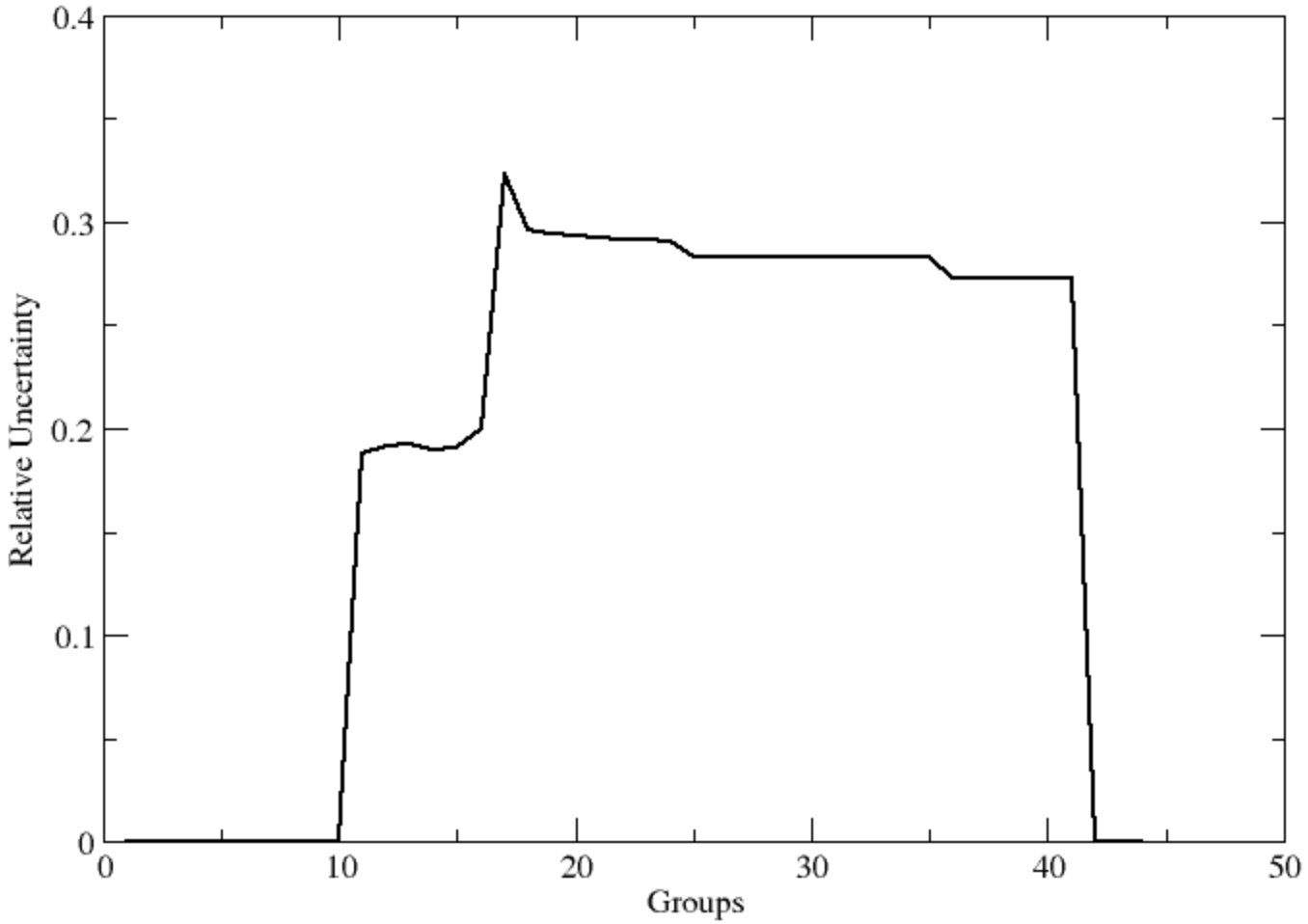
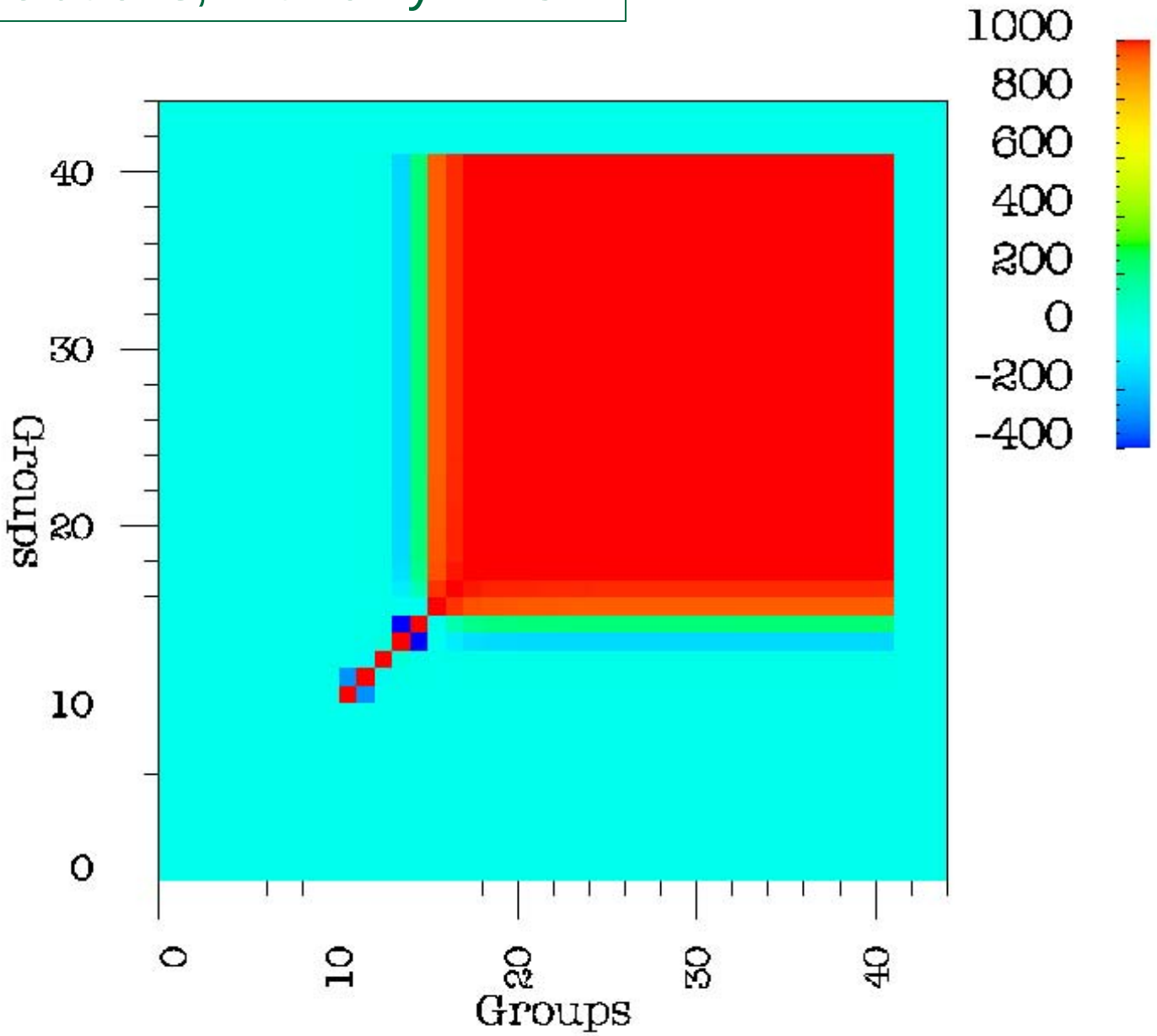
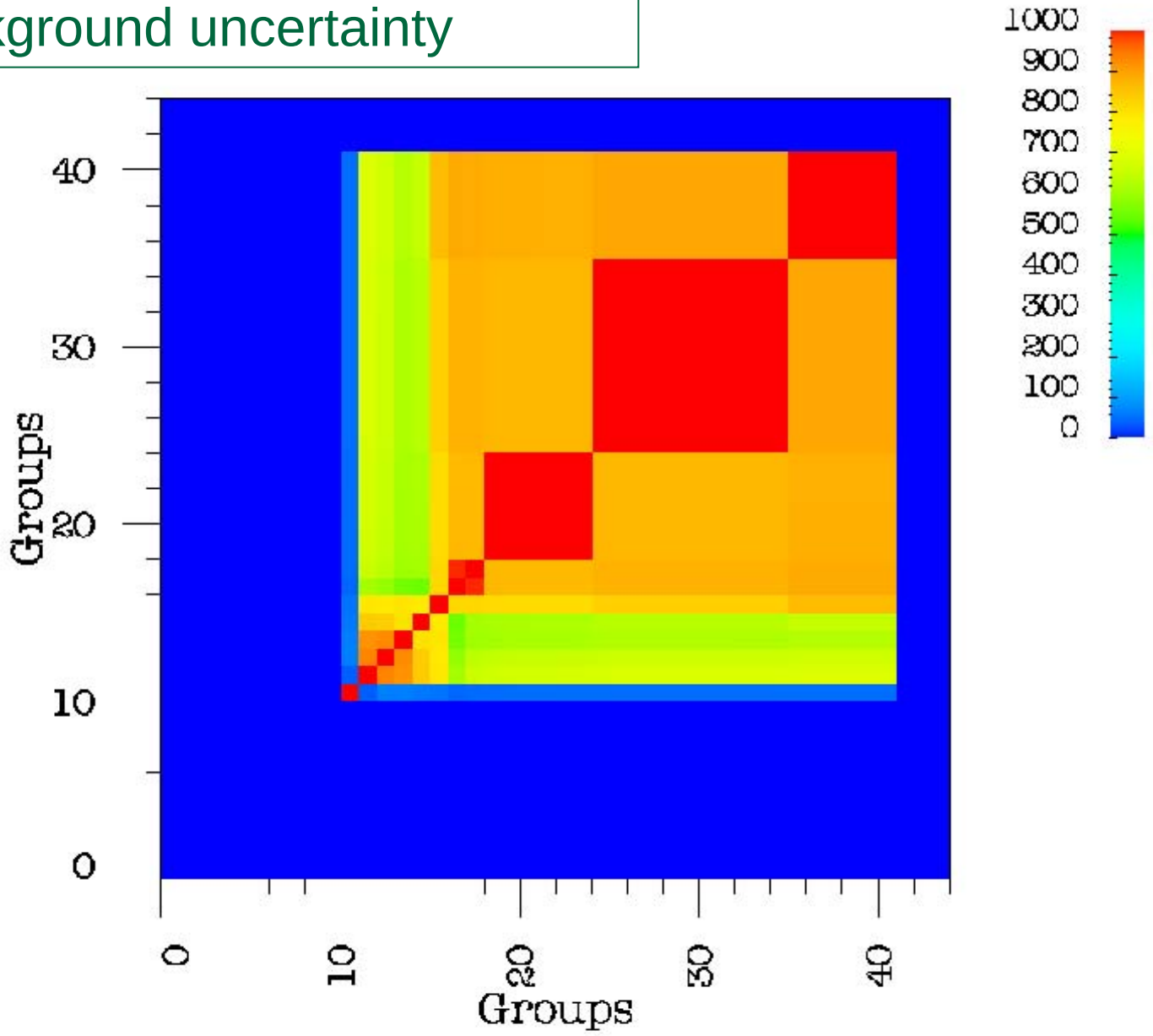
Relative uncertainty, with RPCM + norm + background unc.



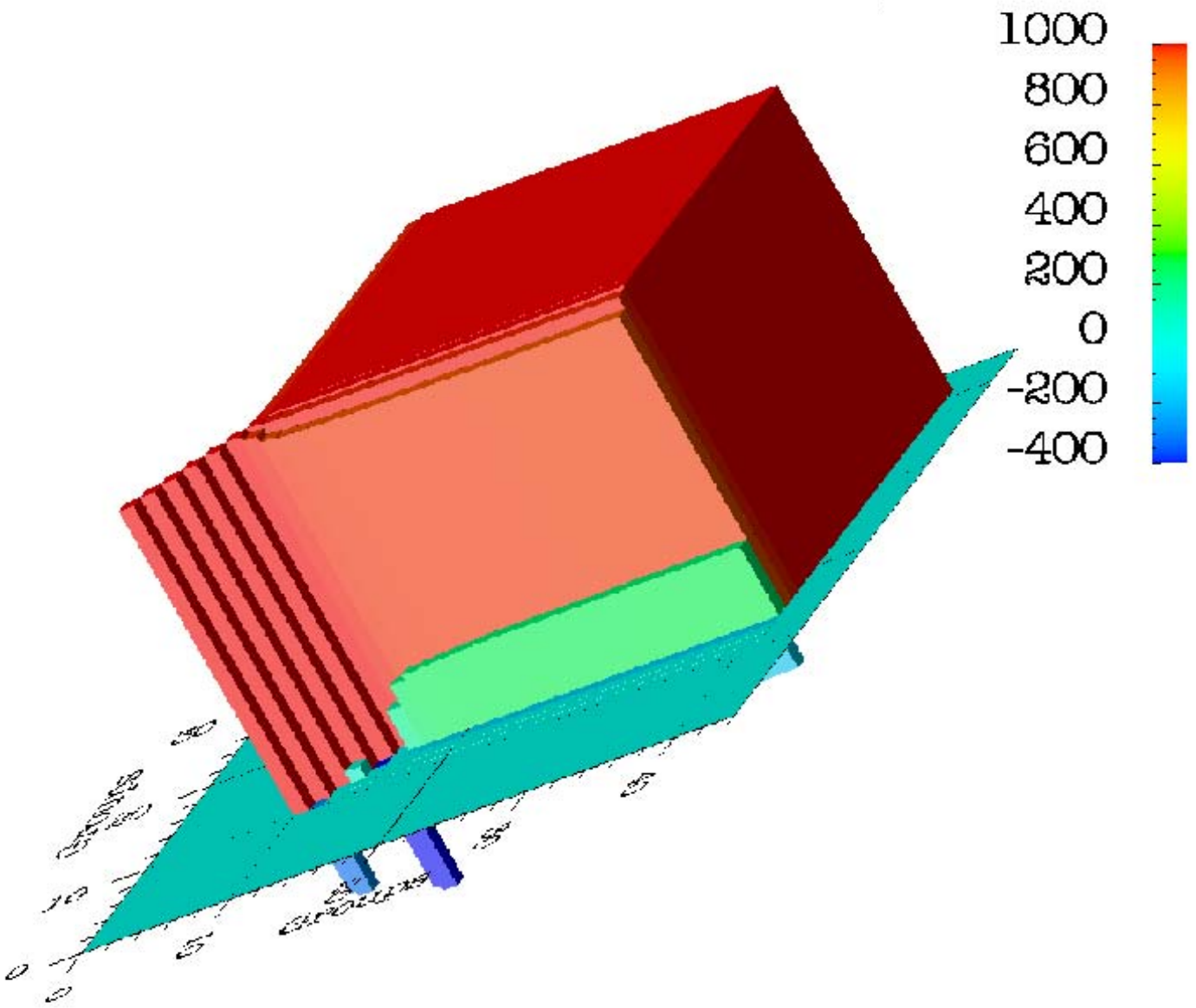
Correlations, with only RPCM



Correlations with RPCM + norm + background uncertainty



Another view of correlations with only RPCM



Another view of correlations with RPCM + norm + background unc.